

BW0	-0.88	-0.70	-0.63
VFpls	0.00	0.00	0.00
Hct0	0.00	0.00	0.00
VFthy	0.01	0.01	0.01
VFthyB	0.00	0.00	0.00
VFthyT	0.01	0.01	0.01
VDFT40	-0.28	-0.35	-0.29
VDFT30	0.02	0.01	0.01
QFC0	0.16	0.14	0.12
QCG	0.00	0.00	0.00
QFthy0	0.16	0.14	0.12
Prob_i	0.00	0.00	0.00
Pthy_i	0.01	0.01	0.01
Prob_p	0.00	0.00	0.00
PRBC_p	0.00	0.00	0.00
Pthy_p	0.00	0.00	0.00
PARBCc_p	0.00	0.00	0.00
KunbC_p	0.00	0.00	0.00
VmaxNISF_thy_i	0.64	0.52	0.46
KmNIS_i	-0.64	-0.52	-0.46
VmaxNISF_thy_p	0.00	0.00	0.00
KmNIS_p	-0.93	-0.93	-0.94
VmaxC_Bp	0.00	0.00	0.00
Km_Bp	0.00	0.00	0.00
Abndmax0	0.03	0.03	0.03
Kbind_i	0.01	0.01	0.01
KprodT4F	0.08	0.06	0.05
KprodT3F	-0.06	-0.05	-0.05
KdegT4F	-0.28	-0.22	-0.24
KdegT3F	0.02	0.01	0.01
CLFul	-0.80	-0.66	-0.59
CLFuP	-0.93	-0.93	-0.93
CLuFT4	-0.89	-0.61	-0.58
CLuFT3	-0.02	-0.01	-0.01
PAFthy_i	-0.01	-0.01	-0.01
PAFthy_p	0.00	0.00	0.00
FRT40	1.90	1.55	1.39
FRT30	0.00	0.00	0.00
bT4	0.00	-0.02	-0.08
AobT4	0.00	-0.14	-0.24
pTSHv	-0.38	-0.38	-0.41
KHCG	0.00	0.13	0.08
CT4TAR	0.73	0.59	0.52
TSHTAR	0.00	0.00	0.00
HCGv	0.00	0.13	0.08

BW0	0.58	0.66	0.70
VFpls	0.00	0.00	0.00
Hct0	0.00	0.00	0.00
VFthy	0.00	0.00	0.00
VFthyB	0.00	0.00	0.00
VFthyT	0.00	0.00	0.00
VDFT40	0.09	0.18	0.18
VDFT30	0.00	0.00	0.00
QFC0	0.02	0.00	0.00
QCG	0.00	0.00	0.00
QFthy0	0.02	0.00	0.00
Prob_i	0.00	0.00	0.00
Pthy_i	0.00	0.00	0.00
Prob_p	0.00	0.00	0.00
PRBC_p	0.00	0.00	0.00
Pthy_p	0.00	0.00	0.00
PARBCc_p	0.00	0.00	0.00
KunbC_p	0.00	0.00	0.00
VmaxNISF_thy_i	-0.38	-0.42	-0.42
KmNIS_i	0.38	0.42	0.42
VmaxNISF_thy_p	0.00	0.00	0.00
KmNIS_p	-0.97	-0.97	-0.97
VmaxC_Bp	0.00	0.00	0.00
Km_Bp	0.00	0.00	0.00
Abndmax0	0.01	0.01	0.01
Kbind_i	0.00	0.00	0.00
KprodT4F	-0.01	0.00	0.01
KprodT3F	0.02	0.02	0.02
KdegT4F	0.09	0.10	0.13
KdegT3F	0.00	0.00	0.00
CLFul	0.36	0.42	0.43
CLFuP	-0.97	-0.97	-0.97
CLuFT4	0.22	0.20	0.22
CLuFT3	0.00	0.00	0.00
PAFthy_i	0.00	0.00	0.00
PAFthy_p	0.00	0.00	0.00
FRT40	-1.19	-1.32	-1.33
FRT30	0.00	0.00	0.00
bT4	0.00	0.01	0.05
AobT4	0.00	0.07	0.12
pTSHv	-0.72	-0.69	-0.67
KHCG	0.00	-0.08	-0.06
CT4TAR	-0.87	-0.94	-0.94
TSHTAR	0.00	0.00	0.00
HCGv	0.00	-0.08	-0.06

```

#-----
# medset.R
#
# Translated from "medset.m".
# Author: Paul Schlosser, U.S. EPA, February-August 2017
# Translator: Dustin Kapraun, U.S. EPA, July-August 2017
#
# Script to define a tuning parameter set for median model predictions. See
# Section 3.2.2 of the BBDR Appendix for details on TH parameters.
#-----

# Extract default parameter values needed for calculations below.
MWI = parms[["MWI"]]

# Variables for later use.
idose = 170.2
CT3tar = 1.74

# Model parameters for which default values should be updated.
BT4 = 0.01845          # NOTE: same as default in .model.
AOBT4 = -0.07782
ABNDMAX0 = 17e6         # NOTE: same as default in .model.
CT4TAR = 100.3
FRT40 = 1.03e-4
FRT30 = 2.77e-3
TSHTAR = 1.39
PTSHV = 1                # NOTE: same as default in .model.
PTSHK = 1                # NOTE: same as default in .model.

# Value of a model state variable to be used later.
Abound_i = 15e6 / MWI

# Update the model parameters for which values were provided above.
parms["bt4"] = BT4
parms["AobT4"] = AOBT4
parms["Abndmax0"] = ABNDMAX0
parms["CT4TAR"] = CT4TAR
parms["FRT40"] = FRT40
parms["FRT30"] = FRT30
parms["TSHTAR"] = TSHTAR
parms["ptshv"] = PTSHV
parms["ptshk"] = PTSHK

# Recompute any parameters that may depend on the updated parameters.
parms = initParms(parms)

```

```

#-----
# merrill_fig_8_10.R
#
# Translated from "Merrill_Fig8-10.m".
# Author: Paul Schlosser, U.S. EPA, February-August 2017
# Translator: Dustin Kapraun, U.S. EPA, July-August 2017
#
# This script produces Figure 49 in the perchlorate BBDR appendix, which
# combines data/results in Figures 8-10 from Merrill et al. (2005). Data were
# contained in model scripts that were part of an acslX package received from
# E. Merrill; sources as identified in Figure 49.
#-----

# Run the script "BBDRPreg_params.R", which assigns values to some variables,
# sets values for parameters in the "parms" vec, and sets initial conditions
# for state variables based on a non-pregnancy simulation to steady state.
source("BBDRPreg_params.R")

# Set up a pre-pregnancy steady state simulation.
TSTOP = 49000
GSTART = 50000
parms["GSTART"] = GSTART
CINT = 500
times = seq(from=0, to=TSTOP, by=CINT)

# Recompute any parameters that may depend on the updated parameters.
parms = initParms(parms)

# Run the pre-pregnancy steady state simulation.
out = ode(Y0, times, func="derivs", parms=parms, dllname=dll_name,
           initfunc="initmod", nout=length(Outputs), outnames=Outputs)

# Use the end-of-simulation values of the state variables in "inames"
# as initial values for the next simulation. For all other state
# variables, use the default initial values.
Y0 = initStates(parms, newStates=out[dim(out)][1], inames))

# At time TSDOSE, put a bolus dose PDOSE_S = BDOSE_PS * BW0 * 1.0e6 / MWCL04
# into the perchlorate stomach compartment Astom_p.
TSDOSE = 240
MWCL04 = parms[["MWCL04"]]

# Simulation time for perchlorate bolus dosing studies.
CINT = 2
TSTOP = TSDOSE + 80
times = seq(from=0, to=TSTOP, by=CINT)

#

```

```

# Kamm and Drescher (1973)
#
# Parameters for Figure 8 (Kamm and Drescher, 1973).
BW0 = 80
parms["BW0"] = BW0
parms = initParms(parms)
BDOSE_PS = 9.56      # Bolus perchlorate dose (mg/kg).
PDOSE_S = BDOSE_PS * BW0 * 1.0e6 / MWCL04    # Bolus perchlorate dose (nmol).

# Data frame containing a single perchlorate bolus dosing event.
df_p = data.frame(var=c("Astom_p"), time=c(TSDOSE), value=c(PDOSE_S),
                   method=c("add"))

# Run simulation for Figure 8 (Kamm and Drescher, 1973).
out = ode(Y0, times, func="derivs", parms=parms, dllname=dll_name,
           initfunc="initmod", nout=length(Outputs), outnames=Outputs,
           events=list(data=df_p))
t_idx = match(TSDOSE, out[, "time"])
fig8_model = data.frame(out[t_idx:dim(out)[1], c("time", "Aelim_p")])
fig8_model$time = fig8_model$time - TSDOSE# Time since bolus dose (h).
fig8_model$Aelim_p = fig8_model$Aelim_p * MWCL04 / 1e6 # Amt. eliminated (mg).

# Data for Figure 8 (Kamm and Drescher, 1973).
fig8_data = data.frame(time=c(0, 4, 8, 12, 16, 20, 24, 28, 32, 36, 40),
                        Aelim_p=c(0, 246, 423, 524, 602, 645, 672, 694, 707, 714, 718))

#
# Eichler (1929).
#
# Parameters for Figure 9 (Eichler, 1929).
BW0 = 70
parms["BW0"] = BW0
parms = initParms(parms)
BDOSE_PS = 20      # Bolus perchlorate dose (mg/kg).
PDOSE_S = BDOSE_PS * BW0 * 1.0e6 / MWCL04    # Bolus perchlorate dose (nmol).

# Data frame containing a single perchlorate bolus dosing event.
df_p = data.frame(var=c("Astom_p"), time=c(TSDOSE), value=c(PDOSE_S),
                   method=c("add"))

# Run simulation for Figure 9.
out = ode(Y0, times, func="derivs", parms=parms, dllname=dll_name,
           initfunc="initmod", nout=length(Outputs), outnames=Outputs,
           events=list(data=df_p))
t_idx = match(TSDOSE, out[, "time"])
fig9_model = data.frame(out[t_idx:dim(out)[1], c("time", "Aelim_p")])

```

```

fig9_model$time = fig9_model$time - TSDOSE # Time since bolus dose (h).
fig9_model$Aelim_p = fig9_model$Aelim_p * MWCL04 / 1e6 # Amt. eliminated (mg).

# Data for Figure 9.
fig9_data = data.frame(time=c(0, 4, 8, 12, 24, 48, 72),
                       Aelim_p=c(0, 478, 935, 981, 1262, 1338, 1.34e03))

#
# Durand (1938).
#

# Parameters for Figure 10 (Durand, 1938).
BW0 = 70
parms["BW0"] = BW0
parms = initParms(parms)
BDOSE_PS = 9.07      # Bolus perchlorate dose (mg/kg).
PDOSE_S = BDOSE_PS * BW0 * 1.0e6 / MWCL04    # Bolus perchlorate dose (nmol).

# Data frame containing a single perchlorate bolus dosing event.
df_p = data.frame(var=c("Astom_p"), time=c(TSDOSE), value=c(PDOSE_S),
                   method=c("add"))

# Run simulation for Figure 10.
out = ode(Y0, times, func="derivs", parms=parms, dllname=dll_name,
           initfunc="initmod", nout=length(Outputs), outnames=Outputs,
           events=list(data=df_p))
t_idx = match(TSDOSE, out[, "time"])
fig10_model = data.frame(out[t_idx:dim(out)[1], c("time", "Aelim_p")])
fig10_model$time = fig10_model$time - TSDOSE# Time since bolus dose (h).
fig10_model$Aelim_p = fig10_model$Aelim_p * MWCL04 / 1e6 # Amt. eliminated (mg).

# Data for Figure 10.
fig10_data = data.frame(time=c(0, 1, 2, 3, 7, 11, 24, 48, 72),
                        Aelim_p=c(0, 67, 143, 210, 375, 475, 564, 604, 605))

#
# Plot data and model outputs together.
#

# Plot Figure 8.
plot(fig8_model$time, fig8_model$Aelim_p, type="l", col="red",
      xlim=c(0, 75), ylim=c(0, 1500),
      xlab="Time (h)", ylab="Perchlorate Eliminated in Urine (mg)")
points(fig8_data$time, fig8_data$Aelim_p, type="p", pch=15, col="red")
lines(fig9_model$time, fig9_model$Aelim_p, lty=2, lwd=2, col="green")
points(fig9_data$time, fig9_data$Aelim_p, type="p", pch=16, col="green")
lines(fig10_model$time, fig10_model$Aelim_p, lty=3, lwd=2, col="black")
points(fig10_data$time, fig10_data$Aelim_p, type="p", pch=18, col="black")

```

```
legend("bottomright", c("Model Simulation (9.56 mg/kg)",
    "Data (Kamm and Dreschler, 1973)",
    "Model Simulation (20 mg/kg)",
    "Data (Eichler, 1929)",
    "Model Simulation (9.07 mg/kg)",
    "Data (Durand, 1938)"),
lty=c(1, -1, 2, -1, 3, -1), lwd=c(1, 1, 2, 1, 2, 1),
pch=c(NA, 15, NA, 16, NA, 18),
col=c("red", "red", "green", "green", "black", "black"), bg="white",
pt.cex=1, cex=0.7)
```

```

#-----
# merrill_fig11.R
#
# Translated from "Merrill_Fig11.m".
# Author: Paul Schlosser, U.S. EPA, February-August 2017
# Translator: Dustin Kapraun, U.S. EPA, July-August 2017
#
# This script produces Figure 48 in the perchlorate BBDR appendix, showing
# model simulations of perchlorate PK data shown in Figure 11 of Merrill et al.
# (2005), attributed to "unpublished data, Brabant and Leitolf". Points are
# mean +/- SD digitized from the figure.
#-----

# Run the script "BBDRPreg_params.R", which assigns values to some variables,
# sets values for parameters in the "parms" vec, and sets initial conditions
# for state variables based on a non-pregnancy simulation to steady state.
source("BBDRPreg_params.R")

# Set up a pre-pregnancy steady state simulation.
TSTOP = 49000
GSTART = 50000
parms["GSTART"] = GSTART
CINT = 500
times = seq(from=0, to=TSTOP, by=CINT)

# Recompute any parameters that may depend on the updated parameters.
parms = initParms(parms)

# Run the pre-pregnancy steady state simulation.
out = ode(Y0, times, func="derivs", parms=parms, dllname=dll_name,
           initfunc="initmod", nout=length(Outputs), outnames=Outputs)

# Use the end-of-simulation values of the state variables in "inames"
# as initial values for the next simulation. For all other state
# variables, use the default initial values.
Y0 = initStates(parms, newStates=out[dim(out)][1], inames))

# At time TGDOSE, put a bolus dose PDOSE_G = BDOSE_PG * BW0 * 1.0e6 / MWCL04
# / NING_G into the perchlorate stomach compartment Astom_p. Likewise, put a
# bolus dose of PDOSE_G into the perchlorate stomach compartment Astom_p
# NING_G total times per day (every FING_G hours) for a total of DAYS_G days.
TGDOSE = 240
BDOSE_PG = 12          # Perchlorate dose (mg/kg/d).
FING_G = 6
NING_G = 3
DAYS_G = 14
MWCL04 = parms[["MWCL04"]]

```

```

# Parameters for Figure 11.
BW0 = 84
parms["BW0"] = BW0
parms = initParms(parms)
PDOSE_G = BDOSE_PG * BW0 * 1.0e6 / MWCL04 / NING_G # Dose (nmol/event).

# Daily perchlorate bolus ingestion times.
tz_daily = seq(from=0, to=(NING_G-1)*FING_G, by=FING_G)

# Vector of all perchlorate bolus dose times.
tz = vector("numeric", DAYS_G * length(tz_daily))

# Build a vector to contain the simulation times at which perchlorate bolus
# ingestion occurs.
idx = 1
for (day in seq(1, DAYS_G, 1)) {
  tz[seq(idx, idx+length(tz_daily)-1, 1)] = TGDOSE + (day - 1) * 24 + tz_daily
  idx = idx + length(tz_daily)
}

# Data frame containing perchlorate bolus dosing events.
df_p = data.frame(var=rep("Astom_p", length(tz)), time=tz,
                   value=rep(PDOSE_G, length(tz)),
                   method=rep("add", length(tz)))

# Simulation time for perchlorate bolus dosing study.
CINT = 0.1
TSTOP = TGDOSE + 400
times = seq(from=0, to=TSTOP, by=CINT)

# Run simulation for 2.5th percentile of median clearance.
parms["CLFuP"] = 0.105
parms = initParms(parms)
out = ode(Y0, times, func="derivs", parms=parms, dllname=dll_name,
          initfunc="initmod", nout=length(Outputs), outnames=Outputs,
          events=list(data=df_p))
t_idx = match(TGDOSE, out[, "time"])
model_025 = data.frame(out[t_idx:dim(out)[1], c("time", "CAtot_p")])
model_025$time = model_025$time - TGDOSE# Time since bolus dose (h).
model_025$CAtot_p = model_025$CAtot_p * MWCL04 / 1e6 # Serum conc. (mg/L).

# Run simulation for 50th percentile of median clearance.
parms["CLFuP"] = 0.122
parms = initParms(parms)
out = ode(Y0, times, func="derivs", parms=parms, dllname=dll_name,
          initfunc="initmod", nout=length(Outputs), outnames=Outputs,
          events=list(data=df_p))
t_idx = match(TGDOSE, out[, "time"])

```

```

model_500 = data.frame(out[t_idx:dim(out)[1], c("time", "CAtot_p")])
model_500$time = model_500$time - TGDOSE# Time since bolus dose (h).
model_500$CAtot_p = model_500$CAtot_p * MWCL04 / 1e6 # Serum conc. (mg/L).

# Data for Figure 11.
fig11_data = data.frame(time=rep(c(3.36, 171.4, 341.2, 363.0, 388.2), 3),
concentration=c(15.26, 13.94, 12.63, 6.52, 3.02, 22.83, 28.36, 25.74, 15.84,
8.12, 7.24, 0.11, -0.76, -2.95, -2.51))

#
# Plot data and model outputs together.
# 

# Plot Figure 11.
plot(model_025$time / 24, model_025$CAtot_p, type="l", col="red",
xlim=c(0, 16), ylim=c(-5, 30),
xlab="Time (d)", ylab="Perchlorate Serum Concentration (mg/L)")
lines(model_500$time / 24, model_500$CAtot_p, lty=1, lwd=2, col="blue")
points(fig11_data$time / 24, fig11_data$conc, type="p", pch=18, col="green")
legend("bottomleft", c("Model (2.5th percentile median clearance)",
"Model (50th percentile median clearance)",
>Data (Fig. 11, Merrill et al., 2005)"),
lty=c(1, 1, -1), lwd=c(1, 2, 1),
pch=c(NA, NA, 18),
col=c("red", "blue", "green"), bg="white", pt.cex=1, cex=0.7)

```

ug/d iodide, fT4 (pM), T4 (nM), fT3 (pM), T3 (nM), TSH (mIU/L)  
89.33314514, 10.29773321, 110.700632, 5.530123813, 1.812651694, 1.293  
121.548912, 12.87216651, 126.1472318, 4.30120741, 1.88945897, 1.944  
240.0589294, 9.01051656, 78.52021574, 4.30120741, 1.597591324, 1.081  
188.6027679, 12.87216651, 109.4134154, 4.762051061, 1.244277858, 0.595  
88.36013031, 12.87216651, 108.1261987, 6.451811116, 1.659037144, 1.35  
365.6080627, 9.01051656, 95.25403221, 5.069280162, 1.966266245, 1.278  
279.454895, 9.01051656, 131.2960984, 4.14759286, 1.720482964, 2.864  
187.9754791, 9.01051656, 105.5517654, 4.608436511, 1.659037144, 0.915  
76.25399017, 9.01051656, 97.82846551, 5.837352914, 1.904820425, 1.091  
177.8801727, 11.58494986, 137.7321817, 4.915665612, 2.473194261, 1.045  
107.3312302, 12.87216651, 104.2645488, 5.530123813, 1.966266245, 1.262  
97.87877655, 7.723299909, 114.562282, 5.837352914, 2.242772435, 0.948  
65.04318237, 10.29773321, 88.81794895, 4.608436511, 1.674398599, 1.603  
100.8516693, 12.87216651, 118.4239319, 4.762051061, 2.119880795, 2.483  
58.36700439, 9.01051656, 87.5307323, 4.30120741, 1.490061139, 2.086  
94.76753235, 10.29773321, 106.8389821, 4.30120741, 1.505422594, 0.556  
152.9806824, 9.01051656, 95.25403221, 4.762051061, 1.689760054, 1.224  
117.5390167, 9.01051656, 97.82846551, 4.915665612, 1.781928784, 1.457  
80.74323273, 10.29773321, 91.39238225, 4.608436511, 1.474699684, 1.107  
94.88756561, 10.29773321, 110.700632, 5.222894713, 1.88945897, 1.061  
154.6141357, 9.01051656, 100.4028988, 5.990967464, 2.25813389, 1.027  
840.2666016, 9.01051656, 86.24351565, 4.30120741, 1.612952779, 1.989  
72.47194672, 12.87216651, 145.4554816, 5.069280162, 1.797290239, 1.983  
120.2915726, 11.58494986, 124.8600152, 4.454821961, 1.582229869, 3.419  
142.3302155, 10.29773321, 95.25403221, 5.222894713, 1.797290239, 0.451  
63.48524094, 6.436083257, 99.11568216, 4.608436511, 1.597591324, 0.596  
427.3462524, 10.29773321, 108.1261987, 4.608436511, 1.628314234, 1.7  
357.5411682, 10.29773321, 88.81794895, 5.376509263, 1.766567329, 0.613  
396.2695007, 10.29773321, 118.4239319, 5.069280162, 1.904820425, 2.671  
144.8697052, 9.01051656, 105.5517654, 4.454821961, 1.490061139, 3.282  
258.7312622, 10.29773321, 110.700632, 4.762051061, 1.413253863, 0.66  
1338.157959, 12.87216651, 122.2855819, 4.915665612, 1.382530953, 1.382  
212.9610138, 11.58494986, 124.8600152, 5.530123813, 1.689760054, 1.075  
145.2002716, 10.29773321, 90.1051656, 5.069280162, 1.659037144, 1.389  
123.8283081, 21.88268307, 159.6148648, 7.680727519, 2.749700452, 0.018  
228.9560547, 18.02103312, 127.4344485, 7.834342069, 2.657531721, 0.002  
265.8701477, 6.436083257, 78.52021574, 4.14759286, 1.474699684, 1.445  
284.3703918, 9.01051656, 92.6795989, 4.915665612, 1.597591324, 0.884  
54.9043541, 9.01051656, 72.08413248, 5.376509263, 1.797290239, 0.704  
55.17224503, 9.01051656, 118.4239319, 5.683738364, 2.765061907, 1.82  
114.1955719, 7.723299909, 81.09464904, 4.608436511, 1.551506959, 2.295  
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